RAL IASI MetOp-A TIR Methane v2.0

Product User Guide

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Change Log

Issue	Author	Affected Section	Reason	Date
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Acronyms

Acronym	Description
BT	Brightness Temperature
CEDA	Centre for Environmental Data Analysis
CF	Climate and Forecast
CH_4	Methane
ECMWF	European Centre for Medium-Range Weather Forecasts
GTOPO30	Global 30 Arc-Second Elevation
HITRAN	High-Resolution Transmission Molecular Absorption Database
IASI	Infrared Atmospheric Sounding Interferometer
IDL	Interactive Data Language
METOP	Meteorological Operational satellite programme
NCEO	National Centre for Earth Observation
RAL	Rutherford Appleton Laboratory
RSG	Remote Sensing Group
STFC	Science and Technology Facilities Council
TIR	Thermal Infrared
UTC	Coordinated Universal Time
VMR	Volume Mixing Ratio
XVMR	Column-averaged Volume Mixing Ratio

1 Introduction

1.1 Purpose and Scope

This document is the Product User Guide for the RAL IASI MetOp-A TIR methane v2.0 dataset. It provides users of the dataset with practical information on the file format and content as well as advice on how to correctly interpret the data.

1.2 Background

In 2016, the RAL IASI MetOp-A TIR methane v1.0 dataset (Siddans et al., 2016) was archived with the Centre for Environmental Data Analysis, providing global, height-resolved atmospheric methane data for public use. The optimal estimation based retrieval algorithm used to produce the v1.0 dataset is described in Siddans et al. (2017).

Since the production of the v1.0 dataset, a number of modifications have been made to the RAL IASI methane processor, necessitating a reprocessing of the IASI MetOp-A record. The main processor modifications are as follows:

- Use of temperature, water vapour, and surface spectral emissivity pre-retrieved from an in-house scheme – the Infrared Microwave Sounder (IMS) retrieval (Siddans et al., 2015) – in place of modelled data.
- Use of a latitudinally varying tropospheric methane prior which more realistically represents the methane distribution, particularly in the northern hemisphere
- The addition of a scale factor for 13CH4 to the state vector (please note: this variable is not currently optimised)

The modified IASI methane processor has been used to reprocess the IASI MetOp-A record, and includes the additional years 2016 and 2017. The resulting RAL IASI MetOp-A TIR methane v2.0 dataset contains 10 years (2007-2017) of global methane retrievals.

1.3 Data Availability

The RAL IASI MetOp-A TIR methane v2.0 dataset is intended to become freely available via the Centre for Environmental Data Analysis (CEDA) catalogue.

For processing purposes, each IASI orbit was split into 16 sections, each containing 50 scan lines. The output NetCDF files correspond to the same orbit subsections; 16 files for each IASI timestamp, appended with two sets of digits representing the start and end scan line contained within the file e.g. '000_049' denotes that the file contains scenes from scan lines 0 to 49.

1.4 Filename Format

The filename format adheres to the following naming convention, with the segregators defined as in Table 1:

<institution>-<processing level>-<product>-<sensor>-<additional segregator>-
<IASI orbit start time>Z_< IASI orbit end time >Z_<orbit section>.nc

E.g. ral-l2-ch4-iasi_metopa-tir_ims-20110629021455Z_20110629035654Z_000_049-v0200.nc

Table 1: File name segregator descriptions.

Segregator	Example
Institution	ral
Processing level	l1, l2, l3
Product	ch4
Sensor	iasi_metopa, iasi_metopb
Additional segregator	tir_ims
IASI orbit start time	YYYYMMDDHHMMSSZ
IASI orbit end time	YYYYMMDDHHMMSSZ
Orbit section	000_049,050_099,100_149,150_199,…750_799

1.5 Data Sampling

IASI has a 2200 km swath and measures both day and night. This provides near global coverage twice per day. IASI has 4 detectors, in a 2 x 2 matrix configuration, each of which has a 12 km diameter approximately circular footprint on the ground at nadir. These detectors scan across-track to give 120 (30 x 4) observations across the 2200 km swath.

Processing was carried out using observations from only one of the four IASI detectors, choosing the measurement which had the warmest (supposedly least cloud-affected) brightness temperature (BT) in a window channel at 950 cm^{-1}.

1.6 Data Quality

1.6.1 Pre-Processing Quality Control

Prior to processing, the data have been quality filtered to remove problematic data, e.g. scenes which are too cloudy or have too cold surface temperature. Retrievals which do not converge satisfactorily are also omitted.

IASI scenes strongly affected by cloud were omitted from processing based on the difference in BT between the IASI observation at 950 cm^{-1} and that simulated on the basis of IMS pre-retrieved data (the *a priori* state for a standard retrieval). Scenes were not processed if the BT difference (observation – simulation) was outside of the range -5 to 15 K.

Furthermore, only scenes having a BT larger than 240 K at 950 cm^{-1} were processed, since the retrieval information content is significantly degraded over very cold surfaces. Convergence can also be poor in these conditions, which are often affected by strong near-surface temperature inversions.

1.6.2 Post-Processing Quality Control

Current recommendations are that the following quality control criteria are applied to the v2.0 data before use:

- Retrieval cost (**chim**) < 120
- Retrieved effective cloud fraction (**cloud_fraction**) < 0.2
- Retrieval convergence (**conv**) = 1

2 Data Format

2.1 General

The data is provided in NetCDF format which adheres to CF compliance standard CF-1.6.

Methane mixing ratios are provided in both profile format and as a column-average. The methane profile is given on 12 fixed pressure levels corresponding to geometric altitude (z*) values of 0, 6, 12, 16, 20, 24, 28, 32, 36, 40, 50 and 60 km. Here, z* is related to pressure as follows:

$$z^* = 16(3 - \log_{10} p).$$

The methane column-average is calculated between the surface pressure and 0.01 hPa.

Where data is provided on levels, these should be interpreted as being the *centre* of an atmospheric layer. The pressure across a layer, corresponding to a given grid level l, is therefore defined as follows:

$$\Delta p_l = \left((p_l - p_{l-1}) + (p_{l+1} - p_l)\right)/2,$$

Where p_l is the pressure at level l, and p_{l+1} and p_{l-1} are the pressures at levels above and below the level l respectively. Following this definition, the level defined at 0 km would extend beneath the surface, therefore the 0 km level should be considered to correspond to a half-layer i.e. a layer bounded by the surface (0 km) and half the distance between the surface and the next defined pressure level.

2.2 Data Dimensions

The dataset dimensions are as described in Table 2, below.

Table 2: Dataset dimensions.

Dimension	Description	Value
pdim	Number of retrievals	Up to 1500
nmlev	Number of model levels	50
nrlev	Number of retrieval levels	12
adim	Number of methane retrieval levels for which averaging kernels are reported (only a subset to reduce the output file size)	5
rsfdim	Number of residual scale factors	2
edim	Number of emissivity values	3
apsfdim	Number of a priori scale factor values	1
al1dim	Number of AVHRR radiances	3
vdim	Number of off-diagonals (one half only) of the solution correlation matrix	66

2.3 Global Attributes

Global attributes of the dataset are set as described in Table 3, below.

Table 3: Description of the output NetCDF global attributes.

Global Attribute	Description
creator_email	RAL RSG contact email address
project	Project name (NCEO)
licence	Details of data licence
platform	Satellite platform (MetOp-A)
sensor	Instrument on-board the satellite platform (IASI)
title	Dataset description (IASI offline thermal-IR methane retrievals)
product_version	Product release version (X.XX)
processor_version	Methane processor version (X.XX)
repository_version	Subversion repository number for methane processor IDL code
build_date	Date/time of code build used for processing (YYYY-MM-DDTHH:MM:SSZ)
processing_date	Date/time processing was performed (YYYY-MM-DDTHH:MM:SSZ)
date_created	Date/time NetCDF file was created (YYYY-MM-DDTHH:MM:SSZ)
institution	Creator institute (STFC Rutherford Appleton Laboratory)
input_file	Input IASI L1b file on the CEDA archive
history	Auxiliary retrieval setup information
input_ims_id	IMS pre-retrieval ID
input_ims_file	Input pre-processed IMS L2 file
time_coverage_start	Start date/time of IASI orbit file processed (YYYY-MM-DDTHH:MM:SSZ)
time_coverage_end	End date/time of IASI orbit file processed (YYYY-MM-DDTHH:MM:SSZ)
references	RAL RSG website reference (http://www.ralspace.stfc.ac.uk/remotesensing)
creator_name	RAL IASI products are developed with funding from the UK National Centre for Earth Observation
geospatial_lat_max	Maximum geospatial latitude within file
geospatial_lat_min	Minimum geospatial latitude within file
geospatial_lon_max	Maximum geospatial longitude within file
geospatial_lon_min	Minimum geospatial longitude within file
processing_status	Processing status (nominal)
conventions	CF compliance version (CF-1.6)

2.4 Variable Attributes

Variable attributes of the dataset are described in Table 4, below.

Table 4: Description of the output NetCDF variable attributes. The retrieved methane profile and column, and their associated errors, are highlighted in light blue.

Variable	Units	Description	Dimensions
ak_vmr	1e-6	Averaging kernel for methane profile mixing ratios (ppmv).	pdim, nmlev, adim
ak_xvmr	1e-6	Averaging kernel for methane column-averaged mixing ratio (ppmv).	pdim, nmlev
ap_ch4iso_sf	-	Apriori 13CH4 scaling factor.	apsfdim
ap_ch4iso_sf_err	-	Apriori error on 13CH4 scaling factor.	apsfdim
ap_ch4_vmr	1e-6	A priori dry-air mole fraction of atmospheric methane (ppmv).	pdim, nrlev
ap_ch4_vmr_err	1e-6	A priori error on retrieved dry-air mole fraction of atmospheric methane (ppmv).	pdim, nrlev
ap_ch4_xvmr	1e-6	A priori column-averaged dry-air mole fraction of atmospheric methane (ppmv).	pdim
ap_ch4_xvmr_err	1e-6	Estimated error on the retrieved column-averaged mixing ratio (ppmv).	pdim
ap_cloud_fraction	-	A priori effective cloud fraction.	pdim
ap_cloud_pressure	hPa	A priori effective cloud-top pressure (hPa).	pdim
ap_hdo_sf	-	Apriori HDO scaling factor.	apsfdim
ap_hdo_sf_err	-	Apriori error on HDO scaling factor.	apsfdim

ap_surface_temperature	K	A priori surface temperature (K).	pdim
bt_diff	K	The brightness temperature difference (K) at 12 microns between observations and simulations (based on ECMWF data). Used to initially screen observations for cloud.	pdim
ch4iso_sf	-	Retrieved 13CH4 scaling factor.	pdim
ch4iso_sf_err	-	Estimated error on retrieved 13CH4 scaling factor.	pdim
ch4_vmr	1e-6	Retrieved dry-air mole fraction of atmospheric methane (ppmv).	pdim, nrlev
ch4_vmr_err	1e-6	Estimated error on retrieved methane profile (ppmv).	pdim, nrlev
ch4_vsx		Off-diagonals of the solution correlation matrix for a subset of retrieval levels (as used for averaging kernels).	pdim, vdim
ch4_xvmr	1e-6	Retrieved column-averaged dry-air mole fraction of atmospheric methane (ppmv).	pdim
ch4_xvmr_eql	1e-6	Column-averaged equivalent CH4 (modelled).	pdim
ch4_xvmr_err	1e-6	Estimated error on the retrieved column-averaged mixing ratio (ppmv).	pdim
chim	-	Retrieval cost function value.	pdim
cloud_fraction	-	Retrieved effective cloud fraction.	pdim
cloud_pressure	hPa	Retrieved effective cloud-top pressure (hPa).	pdim
conv	-	Flag indicating retrieval convergence (1=fully converged). Results with other values should be used with more caution.	pdim
day	-	Day of the month (1-31).	pdim
ecmwf_alt	km	Spatially interpolated ECMWF surface altitude (km).	pdim
emis		Modelled surface spectral emissivity at selected wavenumbers.	pdim, edim
emis_wn	cm-1	Wavenumbers for which modelled surface spectral emissivity is provided.	edim
h2o_xvmr	1e-6	Retrieved column-averaged mole fraction of atmospheric water vapour in air (ppmv).	pdim
hdo_sf	-	Retrieved HDO scaling factor (effective HDO amount compared to HITRAN assumed ratio of HDO to main water vapour isotope).	pdim
hdo_sf_err	-	Estimated error on the retrieved HDO scaling factor.	pdim
iasi_alt	km	Surface altitude (km) corresponding to IASI measurement, based on averaging GTOPO30 to 12km resolution and sampling every 0.05 degrees.	pdim
ims_cloud_fraction	hPa	IMS (pre-retrieval) cloud fraction.	pdim
ims_cloud_fraction	hPa	IMS (pre-retrieval) cloud fraction.	pdim
ims_conv	-	IMS (pre-retrieval) retrieval convergence.	pdim
ims_dt1000	K	Surface - 1000m air temperature difference.	pdim
ims_dt2	K	Surface - 2m air temperature difference.	pdim
ims_jx	-	IMS (pre-retrieval) retrieval cost function value (state vector component).	pdim
ims_jy	-	IMS (pre-retrieval) retrieval cost function value (measurement vector component).	pdim
ims_surface_temperature	K	IMS (pre-retrieval) surface temperature (K).	pdim
lat	degrees_north	Latitude (degrees_north).	pdim
lon	degrees_east	Longitude (degrees east).	pdim
mod_plev	hPa	Pressure levels of true state in provided averaging kernels.	nmlev
month	-	Month of the year (1-12).	pdim
n2o_xvmr_eql	1e-6	Column-averaged equivalent N2O (modelled)	pdim
nstep	-	The average number of retrieval steps (number of calls to the forward model).	pdim
pixel_number	-	IASI detector pixel (0-3).	pdim
rad_avhrr_tir	$W/(m^2\ sr\ m^{-1})$	AVHRR L1 (tir) radiances in channels 3b, 4 and 5.	pdim, al1dim
rad_avhrr_vis	$W/(m^2\ sr)$	AVHRR L1 (vis/nir/swir) radiances in channels 1, 2 and 3a.	pdim, al1dim
ret_plev	hPa	Retrieval pressure levels (hPa).	nrlev

ret_plev_ak	hPa	Pressures of retrieval levels (hPa) for which averaging kernels are provided.	adim
rsf	-	Scale factors for the mean fit and across-track residual patterns.	pdim, rsfdim
rsf_err	-	Errors on residual scale factors.	pdim, rsfdim
scan_line	-	Number of scan line (0=start of orbit).	pdim
scan_position	-	Position within scan line (0-29).	pdim
surface_pressure	hPa	Surface pressure (hPa) used in the retrieval.	pdim
surface_temperature	K	Retrieved surface temperature (K).	pdim
sza	degrees	Solar zenith angle (degrees).	pdim
time_in_msec	msec	Time of day in msec since midnight (UTC).	pdim
vza	degrees	Sensor zenith angle (degrees).	pdim
year	-	Year.	pdim

3 Use of Averaging Kernels

Averaging kernels can be applied to model profiles to take into account the *prior* influence and vertical sensitivity of the IASI retrieval when performing comparisons with independent data or models. The profile and column-averaged methane averaging kernels provided in this dataset, **ak_vmr** and **ak_xvmr** respectively (see Table 4), are given in terms of mixing ratio. They provide the sensitivity of the retrieved profile (or total column average) with respect to perturbations in the "true" profile, defined on a relatively fine grid. It should be noted that:

1. methane profile averaging kernels are only provided for the *first 5 retrieval levels* (i.e. for retrieval levels between 0-20 km)
2. since surface pressure varies in real IASI scenes, but averaging kernels are provided on a fixed pressure grid, the averaging kernel will be zero for pressures greater than the surface pressure of the scene (i.e. beneath the real surface level)

Sections 3.1 and 3.2 describe how to apply the averaging kernels to independent data sources. Section 3.3 describes how to convert the averaging kernels for application to an alternative fine grid (e.g. a native model grid).

3.1 Profile Averaging Kernels

Retrieved profiles should be compared to independent data by applying the profile averaging kernels as follows:

$$\boldsymbol{c_{MxI}} = \boldsymbol{c_a} + \boldsymbol{A_f}(\boldsymbol{x_f} - \boldsymbol{a_f}),$$

where:

- $\boldsymbol{c_{MxI}}$ is the expected retrieved methane vmr profile given the model profile.
- $\boldsymbol{c_a}$ is the *a priori* methane vmr profile (**ap_ch4_vmr** in the retrieval output file) for a given retrieved methane profile.
- $\boldsymbol{A_f}$ is the averaging kernel on a fine grid (defined by **mod_plev** in the retrieval output file) for the given retrieved methane vmr profile (**ak_vmr** in the retrieval output file).
- $\boldsymbol{x_f}$ is the model profile interpolated onto the fine grid on which the averaging kernels are defined.
- $\boldsymbol{a_f}$ is the retrieval *a priori* profile (**ap_ch4_vmr** in the retrieval output file) similarly interpolated onto the fine grid on which the averaging kernels are defined.

3.2 Column-Average Averaging Kernels

In a similar manner to comparing profiles, column-averaged mixing ratios can be compared to model values using:

$$c_{MxI} = c_a + \boldsymbol{A_f}(\boldsymbol{x_f} - \boldsymbol{a_f}),$$

where:

- c_{MxI} is the expected retrieved methane column-average vmr given the model profile.

- c_a is the *a priori* methane column-average vmr (**ap_ch4_xvmr** in the retrieval output file) for a given retrieved methane profile.
- $\boldsymbol{A_f}$ is the averaging kernel on a fine grid (defined by **mod_plev** in the retrieval output file) for the given retrieved methane column-average vmr (**ak_xvmr** in the retrieval output file).
- $\boldsymbol{x_f}$ is as defined in Section 3.1.
- $\boldsymbol{a_f}$ is as defined in Section 3.1.

3.3 Interpolating Averaging Kernels

The value of an averaging kernel at a given fine grid level applies to an atmospheric layer, of finite thickness, centred on the grid level in question. The application of averaging kernels in sections 3.1 and 3.2 requires that the model and *a priori* profiles are interpolated onto the fine grid levels on which the averaging kernels are defined in the NetCDF file (**mod_plev)**. However, comparisons can also be made using profiles defined on an alternative fine grid (e.g. a native model grid), provided that a) the differences in layer thickness between the original and new grids are taken into account and b) the new grid is sufficiently fine to ensure that the averaging kernel captures sufficient variation in both the vertical sensitivity of IASI and the methane profile. (We advise against using a grid coarser than the supplied fine grid.)

The procedure to convert an averaging kernel from its original fine grid to a new fine grid is as follows:

1. Normalise the averaging kernel by dividing its value at each grid level by the corresponding grid layer thickness. The boundaries of a layer corresponding to a given grid level are defined as half the pressure difference between the grid level pressure, p_l, and the pressures at the adjacent levels above and below it, p_{l+1} and p_{l-1} respectively, i.e.

$$\Delta p_l = \big((p_l - p_{l-1}) + (p_{l+1} - p_l)\big)/2.$$

   The normalised averaging kernel, $\boldsymbol{A_f}'$**,** for a given retrieval level, k, and fine grid level, l, can therefore be written as:

$$A_{f:kl}' = A_{f:kl}/\Delta p_l$$

2. Interpolate the normalised averaging kernels (for each retrieval level) to the new fine grid levels, linearly in pressure.

3. Multiply the normalised averaging kernel by the layer thicknesses of the new fine grid (defined as in step 1 above, applied to the new fine grid pressures).

Once the averaging kernel has been converted to the new fine grid, on which the model data is provided, the comparison methods described in Sections 3.1 and 3.2 can then be applied directly.

4 General Points

- A number of geophysical variables have been co-retrieved with methane specifically for the purpose of fitting measured spectra in the methane target interval. However, their quality is not sufficient for use in scientific analyses. Accurate and reliable temperature and water vapour data from the same IASI soundings are available from RAL's IMS v1.0 scheme (Siddans et al., 2018), for example.

- Retrievals are more sensitive towards the ground over land, during the day-time.

- Retrievals are not very sensitive near the surface over very cold surfaces (e.g. ice).

- The retrievals seem to exhibit artefacts over desert and in desert dust plumes.

- Retrievals may be subject to artefacts when there is a very high sulphate aerosol load, following volcanic eruptions. For example, artefacts have been noted following the eruptions of Sarychev in 2009 and Calbuco in 2015.

5 Known Issues

It should be noted that there are some inconsistencies in the underlying IASI L1c and IMS L2 data used in the creation of this dataset, which users should be aware of.

5.1 IASI L1c

IASI L1c data used in the creation of the RAL IASI methane v2.0 dataset was obtained from the CEDA archive and is comprised of several different versions of the data, corresponding to changes in the IASI L1 Product Processing Facility (PPF) software version (IASI Level 1 Product User Guide, 2017). These changes have introduced artefacts in the resulting RAL IASI methane v2.0 dataset (most notably v6.5 in May 2013, v7.2 in May 2015, and v7.3 in September 2015) which should be taken into consideration when analysing the data. At the time of writing, a consistent, reprocessed IASI L1c dataset is not available for public use, but is expected to be available in the near future, at which point a new version (v2.0) of IMS data and the RAL IASI methane data set (v2.1) is planned, and the latter will process all four fields-of-view rather than the least cloudy one of each four.

5.2 IMS L2

IMS L2 data was used to provide a) prior information (surface temperature and water vapour profile) and b) initialisation of the radiative transfer model (temperature, water vapour, and surface spectral emissivity). The majority of the RAL IASI methane v2.0 dataset is based on input from the IMS v1.0 dataset archived with CEDA (Siddans et al., 2018); however, two other, unarchived, IMS data versions were also used where archived data was not available. The use of each IMS version is summarised in Table 5. For the period March-May 2014, data from MHS was unavailable, therefore a version of IMS (IMS v1a) was produced which was not dependent on MHS input. At the time of dataset production, AMSU and MHS for 2017 were not available via CEDA, therefore near-real time AMSU and MHS data received via EUMETCAST were used instead.

Dataset	CEDA archive	Input data	Cloud cleared	Period of use
IMS v1.0	Siddans et al. (2018)	IASI, AMSU, MHS	Yes	2007-2016
IMS v1a	-	IASI, AMSU	No	2014 (Mar-May)
IMS v1b	-	IASI, AMSU (NRT), MHS (NRT)	No	2017

Table 5: IMS pre-retrieved data used in the production of the RAL IASI methane v2.0 dataset.

The use of the three different IMS L2 datasets has not been found to produce artefacts in the IASI methane v2.0 retrieval products, however it is mentioned here for completeness.

6 References

IASI Level 1 Product User Guide, EUM/OPS-EPS/MAN/04/0032, v4D, Eumetsat, 19 September 2017.

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